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Uncertainty Assessment of Equations of State with Application to an Organic Rankine Cycle

Jérôme Frutiger^a, Ian Bell^b, John P. O'Connell^c, Kenneth Kroenlein^b, Jens Abildskov^a, Gürkan Sin^a

^a CAPEC-PROCESS Research Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark (DTU), Kgs. Lyngby, Denmark, gsi@kt.dtu.dk

^b Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, United States of America

^c Department of Chemical Engineering, University of Virginia, Charlottesville, United States of America

Abstract:

Evaluations of equations of state (EoS) with application to process systems should include uncertainty analysis. A generic method is presented for determining such uncertainties from both the mathematical form and the data for obtaining EoS parameter values. The method is implemented for the Soave–Redlich–Kwong (SRK), the Peng–Robinson (PR) cubic EoS, and the perturbed-chain statistical associating fluid theory (PC-SAFT) EoS, as applied to an organic Rankine cycle (ORC) power system to recover heat from the exhaust gas of a marine diesel engine with cyclopentane as the working fluid. Uncertainties of the EoS input parameters, including their corresponding correlation structure, are quantified from the data using a bootstrap method. A Monte Carlo procedure propagates parameter input uncertainties onto the process output. Regressions have been made of the three cubic EoS parameters from both critical point matching and vapor pressure and density data, as used for the three PC-SAFT parameters. ORC power uncertainties of 2–5 % are found for all models from the larger data sets. Mean power values for the cubic EoS are similar for both parameter regressions. The mean power from the PC-SAFT EoS is less than for the cubic EoS, with no overlap of the uncertainty distributions.

Keywords:

Uncertainty analysis, parameter correlation, cubic EoS, PC-SAFT, organic Rankine cycle.

1. Introduction

1.1. Uncertainty in equations of state (EoS) and process models

Thermodynamic cycles such as Organic Rankine Cycles (ORCs) and heat pump systems allow for the recovery of waste heat in process industries and converting it into electrical power or supplying heat back into the system. For example, low-temperature waste heat from marine diesel engines can be used to produce electricity to increase the efficiency of the engine and thereby lower fuel costs and CO₂ emissions [1]. In the preliminary and conceptual design phase of new ORCs or heat pumps, process modeling is necessary to plan, analyze and estimate costs for a given application. The proper selection of working fluid is crucial to the performance of the cycle. Screening techniques and Computer Aided Molecular Design (CAMD) have been extensively applied to find appropriate working fluids for thermodynamic cycles [2][3]. In order to evaluate the thermophysical properties (*e.g.*, enthalpy and entropy) of suitable fluids, an appropriate Equation of State (EoS) is used during process simulations [4]. Different families of EoS have been used extensively in modeling thermodynamic cycles, such as forms of the Helmholtz EoS (as implemented in the well-established REFPROP library [5], or alternatively in the CoolProp library [6]), Cubic EoS (such as Peng–Robinson (PR) [7] or Soave–Redlich–Kwong (SRK) [8]) as well as the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) [9]. Typical criteria for the selection of an EoS are goodness-of-fits to data, range of availability of fluid data, limited complexity of model formulation as related to numerical complexity [10], and/or ease of implementation [11]. The study of Kumar *et al.* [11] demonstrated the sensitivity of natural gas compressor efficiencies to EoS modeling. A much less recognized criterion for the choice of an EoS is the influence of the uncertainty of the fluid-specific parameters of the EoS on the respective process model output. The parameters of an

EoS are often determined through fitting to experimental property data (e.g., critical properties, saturation pressures, and liquid densities). These data have associated uncertainties arising from the measurements [12] and how the model incorporates the values [13]. When applying an EoS to a process, these property uncertainties propagate into output uncertainty of the corresponding process model [14]. It is important to distinguish between accuracy [15] and uncertainty [14] in the context of computational models for process design. Accuracy is the difference between the output predicted by the model and experimental measurements of the property or process output. Uncertainty is the range of statistically possible outcomes of the model (usually assumed to be a normal distribution and reported with 95 % confidence). In the preliminary design phase (e.g., of an ORC system) the accuracy of a process model is often unknown as the process has not been physically constructed, so no experimental measurements of process output are available. In the absence of such experimental data, model output uncertainty is a valuable tool to analyze an EoS.

1.2. Uncertainty quantification for EoS

When fitting the property parameters of an EoS to experimental data using non-linear regression methods, the uncertainties of parameters are defined by the parameter covariance matrix. Feistel *et al.* [16] used generalized least squares for parameter regression and propagated the covariance of the input data uncertainties into the calculated values, obtaining the uncertainties of the derived quantities such as the second and third virial coefficients of water. However, developers only rarely provide the covariance matrix for EoS studies. Recently, Frutiger *et al.* [17] presented a Monte Carlo-based methodology to propagate and quantify the impact of property parameter uncertainty on a process model output of an ORC system. Further, this methodology was used to assess and compare the uncertainty propagation for two different types of EoS: Cubic (SRK) and PC-SAFT [18]. The latter study quantified the parameter uncertainty of SRK and PC-SAFT from measured data using a bootstrap method. These EoS parameter uncertainties were then propagated via a Monte Carlo procedure to the output of an ORC model. Variance-based sensitivity analysis allowed for the comparison of the different outcomes of the uncertainty analyses. In particular, the major results were:

- The ORC output uncertainties were dominated by contributions from the EoS departure functions, rather than contributions from ideal gas heat properties.
- The range of the ORC model output uncertainties were smaller for SRK than for PC-SAFT, for the considered ORC application and working fluid [18].

The EoS and its properties were parameterized as recommended in the literature, and its uncertainty was quantified. This means that the SRK EoS parameters were expressed in terms of the critical temperature, T_c , critical pressure, P_c , and acentric factor, ω , so as to ensure the inflection of the critical isotherm at the critical pressure [19] and to (nearly) reproduce the vapor pressure used to obtain the acentric factor. As a consequence, the uncertainties in T_c , P_c , and ω could be determined from measurements of T_c and vapor-pressure data by fitting to an Antoine-equation. The PC-SAFT parameters σ , ε/k , and m were fitted directly to vapor pressure and liquid density data, as suggested by the developers of the EoS [9]. Thus the different approaches to quantifying the uncertainties followed commonly accepted practice in the literature and typical contemporary approaches to EoS application. However, it could not be determined if the different ranges of the output uncertainties were due to differences in the data used for parameter estimation or to the mathematical form(s) or a combination of these. The present study is based on the previous work of Frutiger *et al.* [18]: The property uncertainties are quantified from experimental data and propagated through an ORC model with cyclopentane as a working fluid, providing the ORC net power output for the given application. In particular, we investigate the following items:

- SRK is parameterized by fitting it directly to the same experimental cyclopentane data as PC-SAFT was. This is not the conventional treatment, and a consequence is that the isotherm exhibiting an inflection point will no longer be at the experimental critical temperature/pressure.

- A bootstrap method quantifies the uncertainties of the three parameters (A , B and β - see below), which are then propagated through an ORC model to obtain the ORC output uncertainty.
- The same analysis is made for Peng-Robinson EoS, to analyze the uncertainty propagation of another commonly used cubic EoS and to compare it to SRK and PC-SAFT.
- The sources of uncertainties are investigated in detail to explore whether the data, or the mathematical structure, or both, are of more influence on the output uncertainty.

The paper is structured as follows: (i) the overall methodology as followed by Frutiger *et al.* [18] is outlined; (ii) PC-SAFT, cubic EoS (SRK and Peng-Robinson), as well as the ORC model, are briefly presented; (iii) the results of the uncertainty analysis of cubic and PC-SAFT EoS are compared.

2. Method and Tools

The methodology consists of the major steps given in Table 1 and is based on the work of Frutiger *et al.* [18].

Table 1. Overview of the methodology.

Step 1	Quantification of uncertainties in fluid-specific EoS parameters based on experimental data using Bootstrap method
Step 2	Monte Carlo procedure for input uncertainty propagation to ORC process model output of cubic (SRK and Peng-Robinson) and PC-SAFT EoS
Step 3	Analysis of ORC model output uncertainty distributions

2.1. Quantification of uncertainties in fluid-specific EoS parameters based on experimental data using Bootstrap method

2.1.1. Formulation of EoS

Solving a thermodynamic cycle model requires evaluating conceptual thermodynamic properties (*e.g.*, enthalpies, entropies, fugacities). Enthalpy and entropy have ideal gas contributions and a non-ideal gas contribution (departure function) [25]. Fugacities are directly calculated from EoS departure functions, or more generally from derivatives of the Helmholtz energy. In this study we compare departure functions from cubic and from SAFT-type EoS: Soave-Redlich-Kwong (SRK) EoS, Peng-Robinson EoS and the non-associating Perturbed Chain Statistical Association Fluid Theory (PC-SAFT) EoS. The ideal gas enthalpy and entropy are obtained for all EoS by integrating the ideal gas heat capacity function as described by Aly and Lee [20]. The uncertainties in the ideal gas contributions were described in the work of Frutiger *et al.* [18]. These are not analyzed here.

PC-SAFT is based on a statistical thermodynamic theory for fluids with a repulsive core and directional short-range attractive sites. A temperature-dependent hard-sphere diameter $d(T)$ for the segments is used to describe the soft repulsion of molecules [21]

$$d(T) = \sigma \cdot [1 - 0.12 \cdot \exp(-3\epsilon / (kT))] \quad (1)$$

with σ as the segment diameter (size parameter), ϵ as the depth of the intersegment molecular pair potential (energy parameter, often reported as ϵ/k), and k as the Boltzmann constant. Further, the non-ideal Helmholtz energy, A_{res} , of a system of N chain molecules has the form

$$\frac{A_{\text{res}}}{NkT} = \frac{A_{\text{hc}}}{NkT} + \frac{A_{\text{disp}}}{NkT} \quad (2)$$

with A_{hc} being the hard-chain reference contribution and A_{disp} being the dispersion contribution. Details of the thermodynamic properties of PC-SAFT can be found in the work of Gross *et al.* [9]. In general, the PC-SAFT EoS is always expressed in terms of the parameters σ (segment diameter),

ϵ/k (energy parameter), and m (chain length parameter). In the work of Frutiger *et al.* [18], the uncertainties of the PC-SAFT parameters σ , ϵ/k , and m were obtained through fitting to collected experimental data for vapor pressure [22] over the temperature range of 230-350 K and saturated liquid densities [23] for a temperature range of 190-310 K using a Bootstrap method (see next section). The uncertainties in σ , ϵ/k and m were afterwards propagated through an ORC model system to obtain the uncertainty of the ORC model outputs (*i.e.*, the net power output uncertainty). The 3-parameter cubic EoS can be written in the following general form,

$$P = \frac{RT}{V_m - b} - \frac{a\alpha(T)}{V_m^2 + (c+1)V_m b - cb^2} \quad (3)$$

with T being the absolute temperature, P the absolute pressure, V_m the molar volume and R is the universal gas constant. The parameters a , b and c as well as the temperature-dependent function $\alpha(T)$ are specific for the particular version of the cubic EoS [25]. For SRK [8] a , b , c and $\alpha(T)$ are given by

$$a = \frac{0.42747R^2 T_c^2}{P_c} \quad (4)$$

$$b = \frac{0.08664RT_c}{P_c} \quad (5)$$

$$c = 0 \quad (6)$$

$$\alpha(T) = \left(1 + (0.480 + 1.574 \cdot \omega - 0.176 \cdot \omega^2) \cdot (1 - \sqrt{T_r})\right)^2 \quad (7)$$

The expressions for a , b and $\alpha(T)$ are developed to guarantee the inflection of the critical isotherm at the critical pressure while T_r is the reduced temperature. The parameters for Peng-Robinson [24] EoS can be similarly expressed as

$$a = \frac{0.45724R^2 T_c^2}{P_c} \quad (8)$$

$$b = \frac{0.077796RT_c}{P_c} \quad (9)$$

$$c = 1 \quad (10)$$

$$\alpha(T) = \left(1 + (0.375 + 1.542 \cdot \omega - 0.270 \cdot \omega^2) \cdot (1 - \sqrt{T_r})\right)^2 \quad (11)$$

In the work of Frutiger *et al.* [18], the property parameter uncertainties in T_c , P_c and ω have been determined and subsequently propagated through the EoS and the process model to the ORC model outputs. For T_c , measurement uncertainty [25][26] served as input uncertainty to the EoS. P_c and ω were obtained using a Bootstrap method to fit vapor pressure to an Antoine equation as described by Patel and Ambrose [27][25]. In this work, we wish to fit the cubic EoS to the same experimental data as used previously for the PC-SAFT EoS and to quantify its uncertainty using a Bootstrap method. This allows comparison uncertainties in the data fitting. To do this, we re-parameterize the two cubic EoS in terms of their parameters a and b as well as a third parameter β . For SRK the re-parameterized EoS is given by

$$P = \frac{RT}{V_m - b} - \frac{a\alpha(T)}{V_m^2 + V_m b} \quad (12)$$

$$\alpha(T) = \left(1 + \beta \cdot \left(1 - \sqrt{T_r}\right)\right)^2 \quad (13)$$

A similar formulation was used for Peng-Robinson EoS. In this way we do not ensure the isotherm with an inflection to be at the critical temperature; instead we consider a , b and β as fluid-specific parameters that should be obtained by fitting the EoS to experimental data. The result is the same number of regressed parameters for all of the EoS models.

2.1.1. Quantification of EoS parameter uncertainty using bootstrap method

The uncertainties and the correlation matrix of the corresponding EoS property parameters are from thermodynamic property data of Daubert [26]. The detailed description and mathematical formulation of the uncertainty quantification can be found in the work of Frutiger *et al.* [18]. The bootstrap method as described by Efron [28] is used. The method quantifies the underlying distributions of residual errors commonly defined in statistical contexts as the differences between the experimental data and their corresponding model calculations. The residual errors are then used to produce synthetic data sets for use in parameter estimation by using random sampling with replacement. In the current study, uncertainties in the PR and SRK EoS parameters were obtained by fitting the EoS to experimental data and carrying out a bootstrap method to obtain the parameter distribution. Vapor pressures [22] over the temperature range of 230-350 K and saturated liquid densities [23] for a temperature range of 190-310 K of cyclopentane have been used. The key steps of the bootstrap methods are the following:

1. A reference parameter estimation is carried out using a non-linear least-squares method to obtain the first parameter estimates.
2. The residual error (*i.e.*, the difference between the experimental and predicted value) for each data point is calculated.
3. New synthetic data sets are produced by *bootstrapping*: residual errors are sampled and added randomly to the estimated properties in the reference step above (*i.e.*, re-arranging the errors).
4. The least squares parameter estimation is repeated using each synthetic data set.
5. The obtained distribution of parameters is analyzed by interference statistics (mean and standard deviation).
6. Uncertainties of the respective parameters are defined as two standard deviations (2SD) of the distributions obtained by the bootstrap method, which is an engineering standard to account for uncertainty with 95 % confidence.

Figure 1 shows the distributions of the EoS parameters of SRK and Peng-Robinson EoS as obtained from the bootstrap method. The breadths of the distributions are similar with the SRK being slightly broader. Because of the different model constructions, the differences in the distribution of the parameters is to be expected.

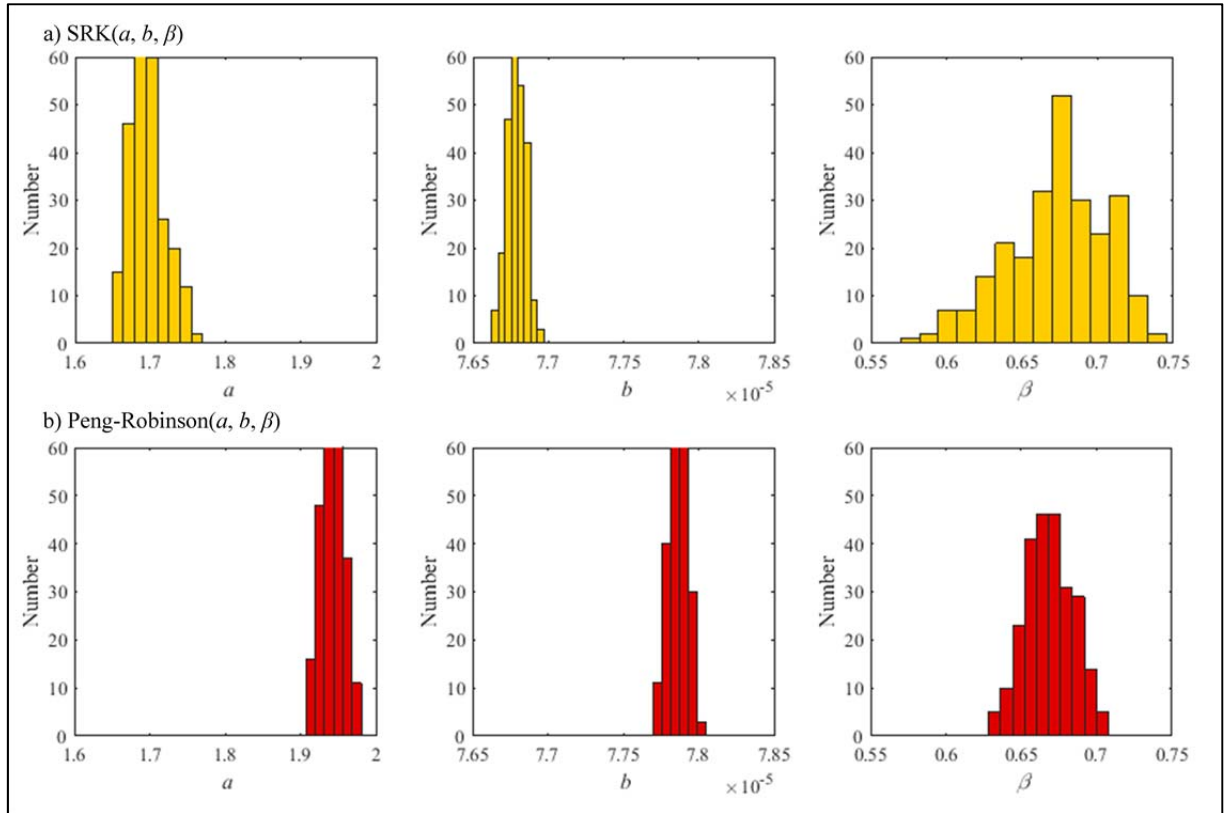


Fig. 1. Distribution of SRK and Peng-Robinson parameters a , b and β obtained from the bootstrap method.

Table 2 summarizes the quantified uncertainty results in a , b and β .

Table 2. Estimated parameters and uncertainties for SRK and Peng-Robinson parameters, respectively. The uncertainties as calculated from the ratio between calculated two standard deviations (SD) and the actual value from the literature.

		a	b	β
SRK	Ref. values [26]	1.72	8.17×10^{-5}	0.78
	Mean values of distribution	1.70	7.69×10^{-5}	0.67
	Uncertainties	2.72 %	0.16 %	9.80 %
		a	b	β
Peng-Robinson	Ref. values [26]	1.84	7.34×10^{-5}	0.66
	Mean values of distribution	1.94	7.79×10^{-5}	0.67
	Uncertainties	1.56 %	0.68 %	4.87 %

2.2. Uncertainty propagation of fluid-specific EoS parameters through ORC model

2.2.1. ORC process formulation

The quantified parameter uncertainties of the corresponding EoS are propagated through an ORC application for power generation using a low-temperature heat source of exhaust gas from a marine diesel engine. Cyclopentane is the working fluid. The process model is based on the work of Andreasen *et al.* [29]. The detailed model description and equations can be found in Frutiger *et al.*

[17][18]. Figure 2 gives an overview over the system containing the components and the corresponding modeling constraints of the process and of the hot fluid.

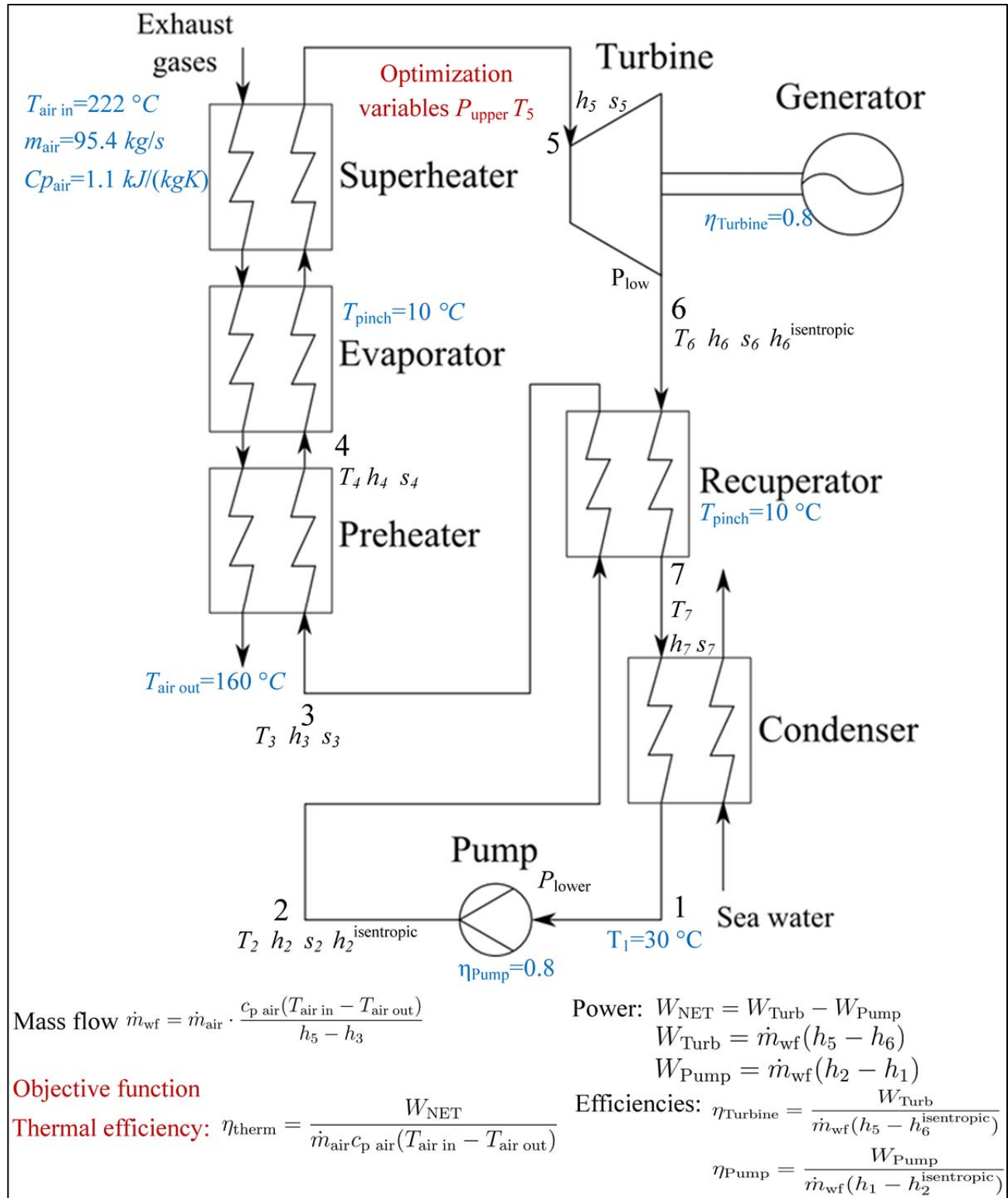


Fig. 2. An overview over the ORC process adapted from Frutiger *et al.* [18]. The objective function is the thermal efficiency η_{therm} , which is optimized subject to the objective variables P_{high} and T_5 and the specified process parameters.

The ORC layout has five main components: pump, evaporator (preheater, evaporator and superheater), turbine, condenser, and recuperator. The outputs from the ORC process model are the net power output W_{NET} , the mass flow \dot{m}_{wf} of the working fluid, and state variables such as

pressures P_i , temperatures T_i , entropies s_i , and enthalpies h_i , (see Figure 2). According to a degrees-of-freedom analysis of the cycle, two process variables can be solved for and optimized. The turbine inlet pressure, $P_5 = P_{\text{high}}$, and the turbine inlet temperature, T_5 have been selected. The optimal process conditions were identified by optimization for cyclopentane.

2.2.2. Monte Carlo procedure for parameter uncertainty propagation through ORC model output of cubic (SRK and Peng-Robinson) and PC-SAFT EoS

A Monte Carlo procedure was used to propagate uncertainties in the fluid-specific EoS parameters to the ORC model power output, W_{NET} . The Monte Carlo method is based on the work of Frutiger *et al.* [17][18] and is as follows:

1. Specification of fluid property and parameter input uncertainties: The quantified uncertainties of the fluid parameters serve as input uncertainties to be propagated through the ORC model.
2. Monte Carlo sampling of property and parameter search spaces: Latin Hypercube Sampling method [30] is used for probabilistic sampling of 250 values from the fluid property parameter defined the range of each property parameter uncertainty. The obtained correlations between the respective parameters were taken into account using the rank-based method for correlation control of Iman and Conover [31].
3. Evaluation of ORC model for each property and parameter sample: The ORC model is evaluated for each of the 250 input parameter samples resulting from Step 2.

In the study of Frutiger *et al.* [18], this procedure was carried out for PC-SAFT parameterized in terms of σ , ϵ/k and m and for SRK EoS parameterized in T_c , P_c and ω . Here, the procedure is applied for SRK and Peng-Robinson EoS parameterized in terms of a , b , and β as well as for the Peng-Robinson EoS parameterized in T_c , P_c and ω . The present results can be compared to the previous results.

3. Results and discussion

Figure 3 shows the output distributions of the ORC net power output W_{NET} as obtained from the evaluated Monte Carlo samples. The results of the combined uncertainty propagations of the departure functions of SRK, Peng-Robinson and PC-SAFT EoS are shown in the three parts: The upper subfigure shows the distribution of PC-SAFT parameterized in σ , ϵ/k , and m , along with the cubic EoS (SRK and Peng-Robinson) parameterized in T_c , P_c and ω . The middle and the bottom subfigures depict the distributions of SRK and of Peng-Robinson parameterized in a , b and β . Furthermore, Table 3 shows the mean values of the distributions with their corresponding uncertainties.

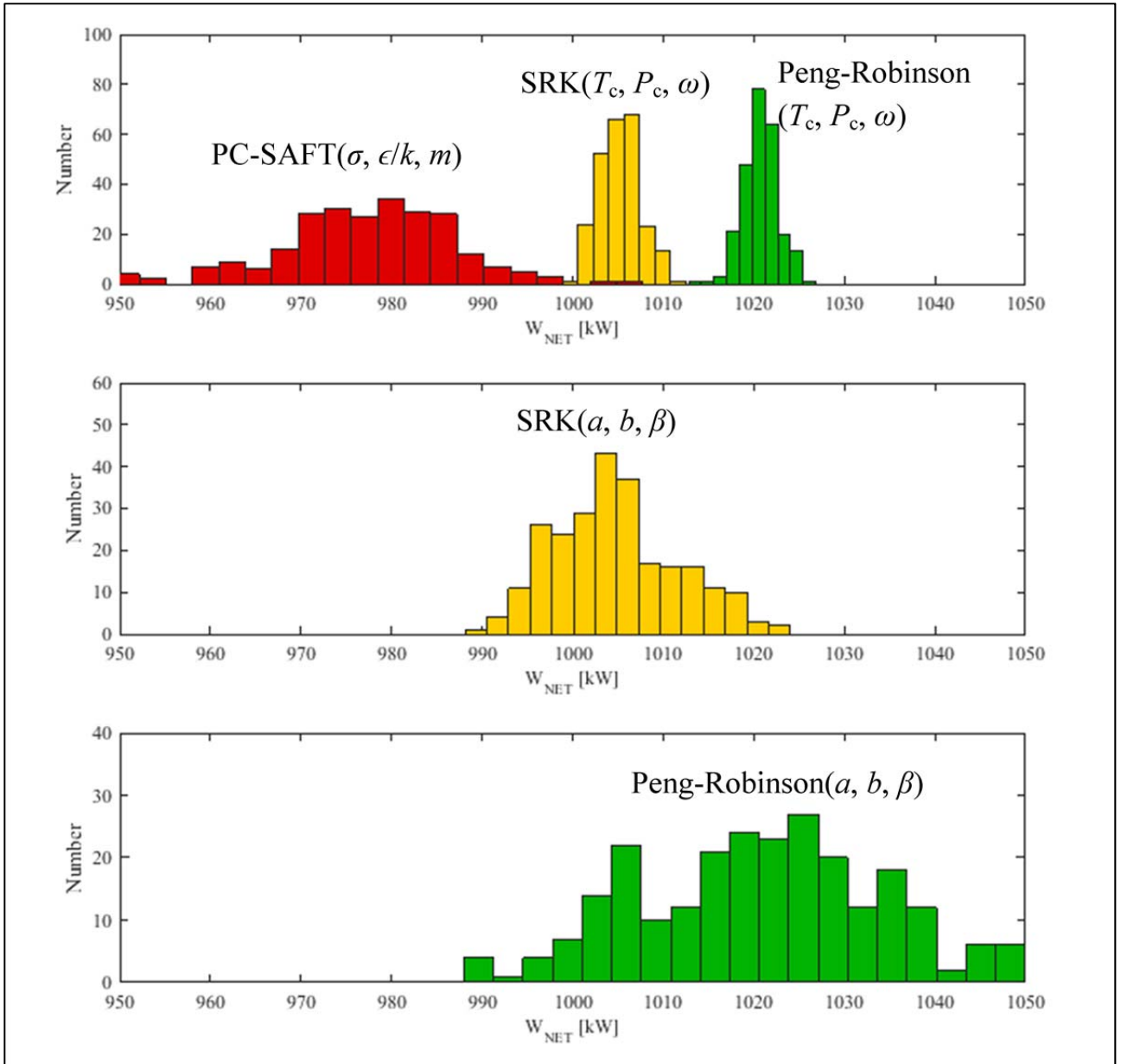


Fig. 3. Output distributions of the ORC net power output W_{NET} from Monte Carlo simulations. The subfigures compare the output distributions of the propagated input uncertainties of the departure functions SRK (yellow), PC-SAFT (red) and Peng-Robinson (green). Distributions of SRK and Peng-Robinson EoS are shown when parameterized in both $(T_c, P_c$ and ω) and $(a, b$ and β).

Table 3. Output uncertainties for W_{NET} subject to the propagation of the respective input uncertainties of SRK, Peng-Robinson and PC-SAFT parameters. The uncertainties as calculated from the ratio between calculated two standard deviations (SD) and the mean value (95 %-confidence). Results from the study of Frutiger et al. [18] are marked with *.

	Mean values of distribution of W_{NET}	Uncertainties
PC-SAFT*	976 kW	1.94 %
SRK (T_c, P_c, ω)*	1005 kW	0.47 %
Peng-Robinson(T_c, P_c, ω)	1021 kW	0.38 %
SRK (a, b, β)	1005 kW	1.36 %
Peng-Robinson (a, b, β)	1020 kW	3.18 %

Figure 3 and Table 3 are revealing in several aspects. First, the two parameterizations of the cubic EoS give different uncertainty distributions. The (a, b, β) forms are much broader than those from (T_c, P_c, ω) , and, similar in breadth to that for the PC-SAFT, are slightly more sharp about the mean. This difference seems to be due to the greater amount of data used in that regression. For practical purposes, the uncertainties in W_{NET} are significant (of the order of 2 – 5 %), and need to be recognized when designing processes such as an ORC. Second, the EoS models give different mean values for W_{NET} with the PC-SAFT giving the lowest by 5 %. There is significant overlap of the distributions only for the (a, b, β) forms of the cubic EoS. Thus, the process results do depend on the model form. Third, the mean values for the cubic EoS are essentially the same for both parameterizations. The later insights suggest that the propagation from properties to mean process outcomes is determined more by model form than by data used in regressions.

4. Conclusions

The uncertainty propagation of different EoS has been investigated for cubic and PC-SAFT EoS. The EoS parameter uncertainties were quantified from measured data using a bootstrap method. The uncertainties were propagated through an ORC cycle model to obtain the uncertainty range of the net power output subject to the uncertainty of the EoS parameters. The common parameterizations of the SRK and PR EoS models yielded somewhat narrower uncertainty distributions than PC-SAFT, with higher net process power values. When the cubic EoS models were reformulated with three regressed parameters, and fitted to the same data as with the PC-SAFT, the uncertainty distributions for power became much broader, though the mean values were quite similar and still greater than those from PC-SAFT. The effects of uncertainties on the power in the example Organic Rankine Cycle are 2-5 %.

Nomenclature

Latin Symbols

A, B	: (In CEOS) adjustable (a, b) -parameters
$A_{\text{res}}, A_{\text{hc}}, A_{\text{disp}}$: Helmholtz energies (residual, hard-chain reference and dispersion)
a, b, c	: CEOS parameters
$d(T)$: (In PC-SAFT): A temperature-dependent hard-sphere diameter
h	: enthalpy
k	: The Boltzmann constant
m	: PC-SAFT parameter (chain length)
\dot{m}_{wf}	: ORC process model mass flow of the working fluid

T	: absolute temperature
T_c	: critical temperature
T_r	: Reduced temperature
P	: absolute pressure
P_c	: critical pressure
R	: gas constant
s	: entropy
V_m	: molar volume
\dot{W}_{NET}	: ORC process model are the net power output

Greek Symbols

ω	: acentric factor
σ	: PC-SAFT parameter (segment diameter)
ε/k	: PC-SAFT parameter (depth of the intersegment molecular pair potential)
β	: (In CEOS) parameter determining T -dependence of a -parameter
$\alpha(T)$: T -dependent factor of Cubic Equations of state
η_{therm}	: thermal efficiency

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